Particle-in-cell Monte Carlo collision simulation of a capacitively coupled discharge in oxygen

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Abstract

The oopd1 particle-in-cell Monte Carlo collision (PIC/MCC) code is used to simulate a capacitively coupled discharge in oxygen. oopd1 is a one-dimensional object-oriented PIC/MCC code in which the model system has one spatial dimension and three velocity components. The oxygen model includes, in addition to electrons, the oxygen molecule in the ground state, the oxygen atom in the ground state, the negative ion O^-, the positive ions O^+ and O_2^+, and the metastable states $O(^1D)$ and $O_2(a^1\Delta_g)$. Here we explore the influence of the metastables $O(^1D)$ and $O_2(a^1\Delta_g)$ on the discharge properties.

Introduction

The oxygen discharge is of vital importance in various materials processing applications such as ashing of photoresist, etching of polymer films and oxidation and deposition of thin film oxides.

Oxygen is a weakly electronegative gas and the presence of negative ions has a strong influence on the kinetics and dynamics of the oxygen discharge.

The oxygen chemistry is rather involved, in particular due to the presence of metastable molecular and atomic oxygen and detachment processes.

The reaction set and cross sections included in the oopd1 code are discussed in the earlier work [1]. Here we add a few reactions involving the metastable oxygen atom $O(^1D)$ and the metastable oxygen molecule $O_2(a^1\Delta_g)$.

Description of the simulation

One of the electrodes is driven by rf voltage

$$V(t) = V_0 \sin(2\pi f t) \tag{1}$$

while the other is grounded.

For this study we assume the discharge to be operated at a single frequency of 13.56 MHz and $V_0 = 222$ V. We assume a large capacitor of 1 F in series with the voltage source.

The diameter of the electrodes is assumed to be 14.36 cm and the gap length between the electrodes 4.5 cm. The discharge pressure is assumed to be 50 mTorr.

The simulation grid is uniform and consists of 1000 cells. The electron time step is chosen to be 3.68×10^{-11} s according to the stability criterion.

The simulation is run for 5500 rf cycles for each case. The density profile and the electron heating rate profile are averaged over 54 rf cycles after the simulation runs to a stable state.

The five cases explored in this study are

- Case 1 – is the basic case explored – the complete reaction set is used that includes both the metastable $O(^1D)$ atom and the metastable $O_2(a^1\Delta_g)$ molecule and the corresponding reactions.
- Case 2 – is the same as case 1 except that the reaction

$$O^- + O_2(a^1\Delta_g) \rightarrow \text{products}$$

  is neglected
- Case 3 – includes the metastable $O(^1D)$ atom and the corresponding reactions
- Case 4 – includes the metastable $O_2(a^1\Delta_g)$ molecule and the corresponding reactions
- Case 5 – includes no metastables

Results and discussion

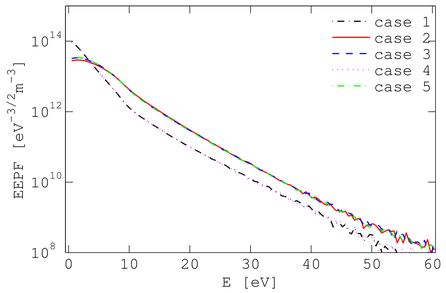

Figure 1: The electron energy probability function (EEPF) in the center of a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm driven by a 222 V voltage source at 13.56 MHz.

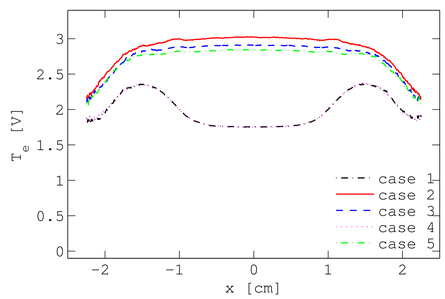

Figure 2: The effective electron temperature profile for a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm driven by a 222 V voltage source at 13.56 MHz.

The electron energy probability function (EEPF) shows a significant change when the metastable singlet oxygen molecule $O_2(a^1\Delta_g)$ is added to the discharge. The number of low energy electrons increases and the number of higher energy electrons (> 10 eV) decreases, the EEPF becomes bi-Maxwellian as seen in figure 1.

Similarly the effective electron temperature decreases significantly, in partcular in the discharge bulk region as seen in figure 2.

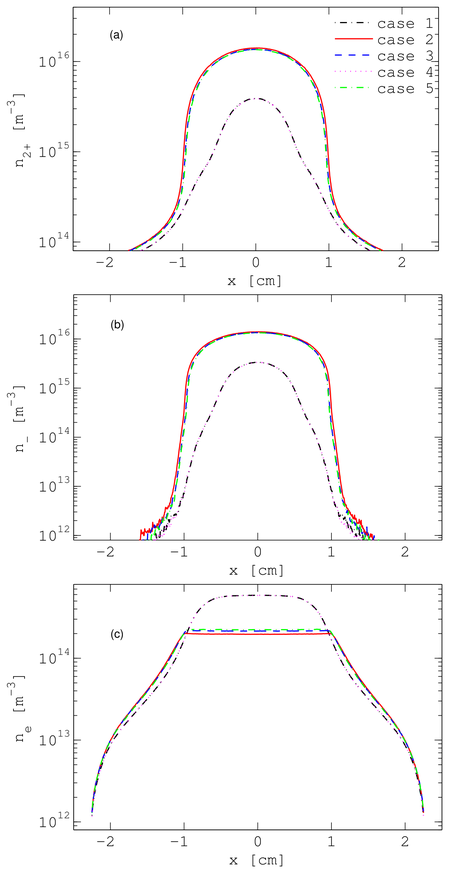

Figure 3: The (a) O_2^+-ion density profile, (b) O^--ion density profile, and (c) electron density profile for a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm driven by a 222 V voltage source at 13.56 MHz.

Figure 3 shows the density profiles for O_2^+-ions, O^--ions, and electrons.

When this detachment process is neglected the O_2^+ and O^- density profiles have the parabolic shape commonly expected from ambipolar drift-diffusion processes in electronegative discharges [2].

The detachment by the metastable singlet oxygen molecule $O_2(a^1\Delta_g)$ has a significant influence on the density profile. The density of O_2^+ and O^--ions is significantly lower and the density of electrons is significantly higher when detachment by the metastable singlet oxygen molecule $O_2(a^1\Delta_g)$ is included in the simulation.

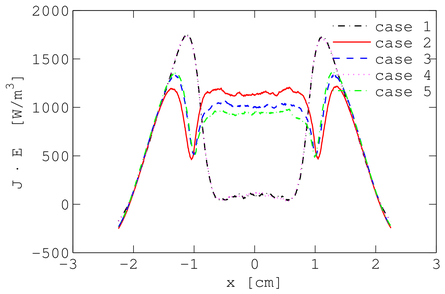

Figure 4: The electron heating rate for a parallel plate capacitively coupled oxygen discharge at 50 mTorr with with a gap separation of 4.5 cm driven by a 222 V voltage source at 13.56 MHz.

This is consistent with the experimental findings of Katsch et al. [3] which claim that the $O_2(a^1\Delta_g)$ is the dominant loss channel for negative ions in a capacitively coupled oxygen discharge. Similar findings were reported by Bronold et al. [4] using particle-in-cell Monte Carlo simulation.

The electron heating mechanism changes from having significant bulk heating to almost entirely sheath oscillation heating when when detachment by the metastable singlet oxygen molecule $O_2(a^1\Delta_g)$ is included in the simulation.

Conclusions

- The influence of the metastable singlet oxygen molecule $O_2(a^1\Delta_g)$ in a low pressure capacitively coupled oxygen discharge is explored and found to be significant.
- In particular detachment by $O_2(a^1\Delta_g)$ is found to be very effective in destroying negative O^--ions in the electronegative core.

References

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